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A LINEARIZED SOLUTION TO IMPULSIVE LATENT HEAT RELEASE IN A DILUTE, ISOTHERMAL ATMOSPHERE

IGOR J. EBERSTEIN KENNETH D. SHERE



JULY 1971



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by

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Part of the research was performed while the author was a

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July 1971

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GODDARD SPACE FLIGHT CENTER

Greenbelt, Maryland

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ABSTRACT

A study is made of the behavior of chemically generated waves in a simplified atmosphere. The atmosphere is assumed unbounded, isothermal, one-space-dimensional and initially quiescent. At an initial time a dissociation reaction, $AB + J \rightarrow A + B + J$, commences and drives the subsequent wave motion. The fraction of reactant in the atmosphere, X_0 , is assumed to be small. The system of governing equations is then expanded in terms of the small parameter, X_0 , and an asymptotic integral solution as $X_0 \rightarrow 0$ is obtained.

The solution is integrated numerically for several natural impulsive heat releases, including thunderstorms, hurricanes, chemical reactions, and aurorae.

Strong thunderstorms and hurricanes are found to induce considerable vertical motion and large temperature changes in the upper atmosphere. The same is true for auroral heat releases. Conversely, upper atmosphere effects of changes in the ozone layer appear to be small.

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A LINEARIZED SOLUTION TO IMPULSIVE LATENT HEAT RELEASE IN A DILUTE, ISOTHERMAL ATMOSPHERE

I. INTRODUCTION

Waves in a stratified fluid under the influence of gravity appear to have been initially discussed by Burnside (1889) and Love (1891). Both authors treated an incompressible fluid. Görtler (1943) used schlierin photography to show experimentally that disturbances in an incompressible stratified medium under the influence of gravity propagate along characteristic rays. Lamb (1908) treated a compressible, adiabatic, ideal gas whose density is stratified by gravity. Since the original contributions by Burnside, Love and Lamb there have been many theoretical papers on various types of gravity waves. Reasonably up-to-date treatments of the subject may be found in Eckart (1960) and Yih (1965). However, gravity wave theory is currently undergoing an active phase of development and contributions are being added to the literature at a rapid rate.

Recent experimental data from the earth's atmosphere and oceans have greatly stimulated interest in gravity-acoustic waves. Gossard (1962) has observed gravity waves in the troposphere. Hines (1960) has shown that internal atmospheric gravity waves may account for many of the phenomena observed

in the lower ionosphere, and gravity waves have been observed in the thermosphere by Newton et. al., (1969) and Harris et al., (1969).

It seems to be generally agreed that gravity waves are generated in the troposphere, then propagate upwards. Thus Gossard (1962) has observed gravity waves near the earth's surface and Eberstein (1970) has illustrated the development of gravity waves between 30 km and 120 km.

The simpler forms of gravity wave theory treat propagation through an inviscid, non-conducting gas, while more sophisticated theories include effects of heat transfer, viscosity, and high altitude phenomena such as ion drag. However, the effect of chemical reactions does not seem to have been adequately considered to date.

Between the troposphere and the thermosphere there are several regions where important chemical reactions take place.

First, there is the ozonosphere between approximately 15 km and 45 km, with peak ozone concentration at about 35 km. Ozone mole fraction is in the order of parts per million (Mitra, 1952).

Between 60 km and 96 km there is Nitric Oxide (Pearce, 1969). The mixing ratio for Nitric Oxide is also in ppm.

Between 90 km and 120 km molecular oxygen dissociates into atomic oxygen. The dissociation ratio, a being 3×10^{-8} at 90 km and 0.998 at 120 km (Mitra, 1952). The oxygen is no longer a truly dilute reactant since its mixing ratio is 20%. However, the high mixing ratio of oxygen becomes a problem only where the final fraction dissociated becomes large. Otherwise, one may use the mathematical expedient of considering only those oxygen molecules which ultimately will dissociate.

The major chemical systems are tied to the absorption of ultraviolet radiation from the sun, and thus have a dawn and dusk dependence. There is also a dependence on solar activity. The latter dependence is more important for the present study, since we are primarily concerned with impulsive heat release or absorption. Periodic thermal effects are in the realm of tidal theory which has been extensively treated in the literature.

Large storms and such phenomena as aurorae may also be simulated by a chemical type heat release.

In what follows, a study is made of the effects on the atmosphere of impulsive heat release in a limited altitude range in a dilute, isothermal atmosphere. A chemical reaction is used as the heat release mechanism, and simplifying assumptions are introduced to make the mathematics more tractable, and permit an anlytical solution. Our objective is a relatively simple theory which may be readily used to study the overall atmosphere effects of large classes of

natural impulsive heat releases. It is recognized that comprehensive numerical techniques have been developed to study the atmospheric effects of impulsive heat release from a point source. However, complicated computer programs are neither generally accessible nor readily modified for general scientific use. Thus we feel that a simple theory of the effects of impulsive heat release in the atmosphere could be helpful in spite of limitations imposed by simplifying assumptions.

II. GOVERNING EQUATIONS

The continuity and momentum equations (cf. Shere and Bowhill, 1969) are not affected by the chemical reaction provided that the state variables are given the extended definition:

$$P = P(\rho, T, \alpha)$$

where P, ρ , T and α denote pressure, density, temperature and degree of advancement of the reaction, respectively. These equations are in tensor notation:

$$\frac{\mathrm{D}\rho}{\mathrm{Dt}} + \rho \frac{\partial \mathrm{u}_{i}}{\partial \mathrm{x}_{i}} = 0$$
 (2.1)

and

$$\rho \frac{Du_{i}}{Dt} = \rho g_{i} - \frac{\partial P}{\partial x_{i}} + \frac{\partial \sigma_{ji}}{\partial x_{j}} \quad (i = 1, 2)$$
 (2.2)

where

$$\sigma_{ji} \equiv \mu \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right]$$

We denote time, space variable (x_2 vertical), velocity component, gravitation vector component, viscous stress tensor, dynamic viscosity and the Kronecker delta by t, x_i , u_i , g_i , σ_{ji} , μ and δ_{ij} respectively. We also take $g_i = -g \delta_{i2}$ and we define D/Dt to be the total or Eulerian derivative.

In order to develop the energy equation, it is necessary to consider the thermodynamics of the system. The derivation of the equation of state parallels the work of Liepmann and Roshko (1957, p. 29) and the derivation of the reaction rate equation parallels the work of Eberstein (1966). The following discussion applies to the reaction

$$J + AB = A + B + J$$

where J is an inert element. We assume that each component of the mixture is a perfect gas. The mixture, however, is not a perfect gas. The partial pressure of the ith constituent is

$$P_i = m_i \rho R_i T \tag{2.3}$$

where $R_i = \Re/W_i$ with \Re the universal gas constant, W_i the molecular weight, and m_i the mass fraction of ith-component. Letting α be the fraction of AB dissociated, n_i the number of moles of ith component, and n_0 the total number of moles when $\alpha = 0$,

$$n_{AB} = n_0 X_0 (1 - \alpha)$$
 $n_A = n_0 X_0 \alpha$
 $n_B = n_0 X_0 \alpha$
 $n_J = (1 - X_0) n_0$
(2.4)

where X_0 is the mole fraction of AB when $\alpha = 0$. Summing yields

$$\Sigma n_i = n_0 (1 + \alpha X_0).$$

$$P = R(\alpha) \rho T \qquad (2.5)$$

$$R(\alpha) = \Re / M$$

where \Re is the universal gas constant, and M is the mean molecular weight, given as:

$$\mathbf{M} = \left[\mathbf{W}_{\mathbf{J}} + \mathbf{X}_{\mathbf{0}} \left(\mathbf{W}_{\mathbf{A} \mathbf{B}} - \mathbf{W}_{\mathbf{J}} \right) \right] / \left[\mathbf{1} + \alpha \mathbf{X}_{\mathbf{0}} \right]$$

It follows that

$$R(\alpha) = R(0) (1 + \alpha X_0)$$
 (2.6)

The reaction equation is as follows:

$$Dn_{AB}/Dt = -\left\{k_{F}(T)\left[\frac{n_{AB}}{V}\right] - k_{B}(T)\left[\frac{n_{A}}{V}\right]\left[\frac{n_{B}}{V}\right]\right\}N \qquad (2.7)$$

where

$$N = \sum_{i=1}^{n} n_{i}$$

and k is a rate constant. In determining (2.7) it has been implicitly assumed that all molecules present may act as an inert element with equal collision effectiveness. Substituting (2.4) into (2.7) yields

$$\frac{D\alpha}{Dt} = \left[\rho k_{F}(T)/M\right] \left\{1 - \alpha - \left[K(T)\rho/M\right] \left(\frac{X_{0}\alpha^{2}}{\left[1 + X_{0}\alpha\right]}\right)\right\}$$
 (2.8)

where

$$K(T) = \frac{k_B(T)}{k_F(T)}$$

and M is the mean molecular weight

For chemical equilibrium, the rate equation reduces to

$$\frac{1-\alpha}{\alpha^2} = \frac{P}{K_P} \left(\frac{X_0}{1+\alpha X_0} \right)$$

where use was made of the equality

$$K = K_C = \frac{K_P}{RT}$$

In atmospheric problems the reactant fraction is generally small, and it will be assumed that $X_0 << 1$. It follows that $\alpha X_0 << 1$. The rate equation may thus be simplified to give:

$$\frac{D\alpha}{Dt} = \left[\rho k_F(T)/M \right] \left\{ 1 - \alpha \right\}$$
 (2.9)

The energy equation is now developed in the usual manner (cf. Liepmann and Roshko, 1957, p. 185+). Summing the rate of change of the internal, kinetic and potential energy yields

$$\int_{V}^{\frac{\partial}{\partial t}} \left(\rho e + \frac{1}{2} \rho u_{i} u_{i} + \rho g x_{2} \right) dV$$

$$+ \int_{A} \left(\rho e + \frac{1}{2} \rho u_{i} u_{i} + \rho g x_{2} \right) u_{j} n_{j} dA$$

$$= - \int_{A} P n_{i} u_{i} dA + \int_{A} u_{i} \sigma_{ij} dA + \int_{A} \kappa \frac{\partial T}{\partial x_{i}} n_{i} dA \qquad (2.10)$$

where n_i is the ith component of the unit normal of the closed surface ϕ , V is the volume of ϕ and A the area; e is the internal energy per unit mass and κ is the coefficient of thermal conductivity.

By applying Gauss' theorem and substituting the continuity and momentum equations into (2.10), we obtain

$$\rho \frac{\mathrm{De}}{\mathrm{Dt}} = -\mathrm{P} \frac{\partial \mathrm{u}_{i}}{\partial \mathrm{x}_{i}} + \sigma_{i j} \frac{\partial \mathrm{u}_{i}}{\partial \mathrm{x}_{i}} + \frac{\partial}{\partial \mathrm{x}_{i}} \left(\kappa \frac{\partial \mathrm{T}}{\partial \mathrm{x}_{i}} \right) \tag{2.11}$$

We now use the first law of thermodynamics, $h = e + P/\rho$, and the continuity equation to obtain

$$\rho \frac{Dh}{Dt} = \frac{DP}{Dt} + \sigma_{ij} \frac{\partial u_i}{\partial x_i} + \frac{\partial}{\partial x_i} \left(\kappa \frac{\partial T}{\partial x_i} \right)$$
 (2.12)

In a reacting gas mixture the enthalpy depends on the temperature and the degree of reaction, i.e.

$$h = h(T, \alpha)$$

The rate of change of enthalpy per unit mass is then given by:

$$\frac{Dh}{Dt} = C_p \frac{DT}{Dt} + X_0 B \frac{D\alpha}{Dt}$$
 (2.13)

where B is the enthalpy of reaction and C_p is heat capacity. For an endothermic (exothermic) reaction, B is positive (negative). Both the enthalpy of reaction

and the heat capacity have a weak temperature dependence, and an even weaker pressure dependence. For simplicity both \mathbf{C}_{p} and B will be assumed constant throughout this paper.

Eliminating h between (2.12) and (2.13) one obtains the enthalpy equation in the form:

$$\rho C_{P} \frac{DT}{Dt} + X_{0} B \frac{D\alpha}{Dt} = \frac{DP}{Dt} + \sigma_{ik} \frac{\partial u_{i}}{\partial x_{k}} + \frac{\partial}{\partial x_{i}} \left(\kappa \frac{\partial T}{\partial x_{i}} \right)$$
(2.14)

The independent variables in the system of equations described above are t, x_i . The quantities k_F , K, c_p and B are known parameters of the system, X_0 is a small (known) parameter. The dependent variables are P, ρ , T, u_i , and α .

For the remainder of this paper we assume that the atmosphere is inviscid and nonconducting, i.e., $\kappa = \lambda = 0$

III. NONDIMENSIONALIZATION OF THE GOVERNING EQUATIONS

Since mathematical operations are performed on pure numbers it is proper to non-dimensionalize the governing equations.

Some of the non-dimensionalization is almost trivial, as shown immediately below:

$$R' = R/R(0) \qquad M' = M/M*$$

$$C_{\mathbf{P}}' = C_{\mathbf{P}}/R(0) \qquad k_{\mathbf{F}}' = k_{\mathbf{F}}\rho_{*}/M*\omega_{\mathbf{B}}$$

$$\rho' = \rho/\rho_{*} \qquad K' = K\rho_{*}/M*\omega_{\mathbf{B}}$$

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where R(0) is the gas constant for $\alpha=0$, and the starred reference level is the value at the bottom of the reaction zone. $\omega_{\rm B}$ is a base frequency, and H is scale height

$$t' = t\omega_{B}$$

$$T' = R(0) T/\omega_{B}^{2} H^{2}$$

$$R' = R(0) T/\omega_{B}^{2} H^{2}$$

It is seen that in the primed system we have

In general, the non-dimensional system of governing equations looks very similar to the dimensional system.

The quantity $\omega_B^2 H^2$ is proportional to the energy contained in a wave oscillating with the base frequency, and having amplitude equal to a pressure scale height. The quantity $H\omega_B^2$ is a measure of the acceleration experienced in such a wave. Since such acceleration must be less than that due to gravity we would expect $g^{\dagger} > 1$.

One may estimate the magnitudes of the non-dimensional parameters.

Taking a scale height of 6 km and a base period of 5 minutes, one obtains

$$(\omega_B^{}H)^2 \sim 1.6 \times 10^8 \text{ cm}^2/\text{sec}^2 = 3.74 \text{ calories/gram}$$

and

$$\omega_{\rm B}^2$$
 H ~261 cm/sec², giving ${\rm g'} \sim 3.5$ ${\rm T'} \sim 3.5$

Further, taking B = 34.4 kcal/gmole, M = 48g/gmole, one obtains $B' \sim 200$.

IV. ASYMPTOTIC DEVELOPMENT

The non-dimensionalized system of equations will be expanded about the parameter X_0 , i.e., we expand each dependent variable in a power series of the form:

$$f(t, x, z) = \sum_{N=0}^{\infty} f^{(N)}(t, x, z) X_0^N$$
 (4.1)

where higher order terms may be dropped as $X_0 \to 0$. This expansion limits the validity of our results to dilute fluids, such as the atmosphere. Other expansions [cf. Lax, 1957] can be obtained by inserting a small parameter into the initial conditions. These expansions may, for example, be used to study the generation of gravity waves by tidal waves.

Assume that the atmosphere is initially stratified, quiescent, and bounded below by the earth, i.e., we define an initial-boundary value problem with initial conditions:

$$T(0, x, z) = T_0 = T_*$$

$$u_i(0, x, z) = 0 (i = 1, 2)$$

$$\rho(0, x, z) = e^{-z}$$

$$\alpha(0, x, z) = 0$$
(4.2)

and boundary condition:

$$u_2(t, x, 0) = 0$$

Using the equation of state to eliminate P from the governing equations and substituting (4.1) into the resultant system yields the zero-order solution

$$T^{(0)}(t, x, z) = T_0 = T_*$$

$$u_i^{(0)}(t, x, z) = 0$$

$$\rho^{(0)}(t, x, z) = e^{-z}$$

$$\alpha^{(0)}(t, x, z) = 1 - \exp[-k_F \rho^{(0)} t]$$
(4.3)

Defining $T^{(1)} = T^{(0)} T_{(1)}$; $\rho^{(1)} = \rho^{(0)} \rho_{(1)}$ and $\alpha^{(1)} = \alpha^{(0)} \alpha_{(1)}$, we get the first order system

$$\frac{\partial u_1^{(1)}}{\partial t} + T_0 \frac{\partial \rho_{(1)}}{\partial x} + T_0 \frac{\partial T_{(1)}}{\partial x} = 0$$
 (4.4)

$$\frac{\partial u_2^{(1)}}{\partial t} + T_0 \frac{\partial P_{(1)}}{\partial z} - T_{(0)} T_{(1)} + T_0 \frac{\partial T_{(1)}}{\partial z} = -T_0 \frac{\partial \alpha^{(0)}}{\partial z} + T_0 \alpha^{(0)}$$

$$(4.5)$$

$$\frac{\partial \rho_{(1)}}{\partial t} + \frac{\partial u_1^{(1)}}{\partial x} + \frac{\partial u_2^{(1)}}{\partial z} - u_2^{(1)} = 0.$$
 (4.6)

$$-\frac{\partial \rho_{(1)}}{\partial t} + \frac{1}{\gamma - 1} \frac{\partial T_{(1)}}{\partial t} + u_2^{(1)} = -\beta \frac{\partial \alpha^{(0)}}{\partial t}$$
 (4.7)

$$\frac{\partial \alpha_{(1)}}{\partial t} \alpha^{(0)} + \alpha_{(1)} \frac{\partial \alpha^{(0)}}{\partial t} = \Gamma^{(1)} (\rho^{(0)}, \alpha^{(0)})$$
 (4.8)

where

$$\mathbb{B} = \left(\frac{\mathbf{B}}{\mathbf{T_0}} - \mathbf{1}\right).$$

Equations (4.4) - (4.7) form a linear system of four partial differential equations in four unknown functions. The system is inhomogeneous. The solution of (4.8) for $\alpha_{(1)}$ is needed only for the calculation of second order terms. Since we determine only the first order terms in this paper, we will neither specify $\Gamma^{(1)}$ nor solve for $\alpha_{(1)}$.

Dropping the (1) subscript or superscript and eliminating we obtain the equation

$$\left\{ \frac{\partial^{2}}{\partial t^{2}} \left[\frac{\partial^{2}}{\partial t^{2}} - C^{2} \frac{\partial^{2}}{\partial x^{2}} - C^{2} \frac{\partial^{2}}{\partial z^{2}} + C^{2} \frac{\partial^{2}}{\partial z} \right] - \frac{\gamma - 1}{\gamma^{2}} C^{4} \frac{\partial^{2}}{\partial x^{2}} \right\} T = f\left(\alpha^{(0)}\right) (4.9)$$

where

$$f(\alpha^{(0)}) = -(\gamma - 1) \beta \frac{\partial^2}{\partial t^2} \left[\frac{\partial^2}{\partial t^2} - T_0 \frac{\partial^2}{\partial x^2} - T_0 \frac{\partial^2}{\partial z^2} \right] \alpha^{(0)}$$

$$- (\gamma - 1) B \frac{\partial^{3} \alpha^{(0)}}{\partial t^{2} \partial z} + (\gamma - 1) T_{0}^{2} \frac{\partial^{2} \alpha^{(0)}}{\partial x^{2}} (4.10)$$

and

$$C^2 = \gamma T_0$$

After (4.9) is solved, the other dependent variables can be determined by the equations

$$\left[\frac{\partial^2}{\partial t^2} + T_0 \frac{\partial}{\partial z}\right] \rho = \frac{1}{\gamma - 1} \frac{\partial^2 T}{\partial t^2} - T_0 \frac{\partial T}{\partial z} + T_0 T + B \frac{\partial^2 \alpha^{(0)}}{\partial t^2} + T_0 \alpha^{(0)} (4.11)$$

$$\frac{\partial u_1}{\partial x} = -\frac{\partial^2 \rho}{\partial t \partial z} + \frac{1}{\gamma - 1} \frac{\partial^2 T}{\partial t \partial z} - \frac{1}{\gamma - 1} \frac{\partial T}{\partial t} + B \frac{\partial}{\partial t} \left(\frac{\partial}{\partial z} - 1 \right) \alpha^{(0)}$$
 (4.12)

and

$$u_2 = \frac{\partial \rho}{\partial t} - \frac{1}{\gamma - 1} \frac{\partial T}{\partial t} - \beta \frac{\partial \alpha^{(0)}}{\partial t}$$
 (4.13)

Now define

$$\theta(t, x, z) = e^{-z/2} T(t, x, z)$$
 (4.14)

The above definition allows the temperature perturbation to grow exponentially with altitude without a corresponding growth in θ .

Substituting the definition of θ into (4.9) yields:

$$\frac{\partial^2}{\partial t^2} \left[\frac{\partial^2}{\partial t^2} - C^2 \nabla^2 + \frac{C^2}{4} \right] \theta - \frac{C^2 (\gamma - 1)}{\gamma^2} \frac{\partial^2 \theta}{\partial x^2} = e^{-z/2} f(\alpha)$$
 (4.15)

 $f(\alpha^{(0)})$ was defined in Equation (4.10).

The dispersion equation of (4.15) is:

$$\lambda_{t}^{4} - C^{2} \left(\lambda_{x}^{2} + \lambda_{z}^{2} + \frac{1}{4} \right) \lambda_{t}^{2} + \left[(\gamma - 1) C^{4} / \gamma \right] \lambda_{x}^{2} = 0$$
 (4.16)

where λ_{i} is the wave number of i.

For a discussion of dispersion relations and how these are obtained from partial differential equations reference is made to Courant and Hilbert, especially p. 588.

V. SOLUTION OF THE FIRST-ORDER SYSTEM

From (4.4)-(4.6) and the initial conditions (4.2) we deduce that

$$\theta(0, \mathbf{x}, \mathbf{z}) = 0 \tag{5.1a}$$

$$\theta_{t}(0, \mathbf{x}, \mathbf{z}) = -(\gamma - 1) \, \beta k_{t} \, e^{-3z/2}$$
 (5.1b)

Conditions for $\theta_{t\,t}$ and $\theta_{t\,t\,t}$ at t=0 can be determined by differentiating (4.4)-(4.8) appropriately and analyzing the resultant system or by integrating (4.15) and applying the physical requirement that $\theta(t, x, z)$ must remain bounded as $t\to\infty$. The negativeness of $\theta_t(0, x, z)$ means that the atmosphere initially cools, which is in correspondence with the endothermic reaction indicated by positive β .

Since the inhomogeneous parts of (4.5)-(5.1) do not depend upon the horizontal space variable, neither does the solution. Thus (4.15) reduces to

$$\frac{\partial^2}{\partial t^2} M[\theta] = e^{-z/2} f(\alpha)$$
 (5.2)

where

$$M[\cdot] = \frac{\partial^2}{\partial t^2} - C^2 \frac{\partial^2}{\partial z^2} + C^2/4.$$
 (5.3)

It is worth noting that the initial conditions and the alpha dependence chosen are such as to imply the relevance of only one space dimension. Other initial or boundary conditions would require that the second space dimension be kept. Unfortunately, exclusion of the lateral space dimension removes many interesting physical phenomena from the realm of applicability of the theory. However, it must also be realized that keeping the lateral space dimension is only mearingful if one also knows the horizontal behavior of the forcing function. Otherwise, one can only calculate propagation of waves, but not their generation.

Integrating (5.2) with respect to time twice, $M[\theta] = w(t, z) = k_F(\gamma - 1) \{k_f [-\beta + Bt^2] e^{-z} - 2Bt\} \exp{-\left[\frac{3z}{2} + k_F t e^{-z}\right]}$ (5.4) subject to initial conditions (5.1).

The inhomogeneous part of (5.2) is the effect of the chemical reaction. For a realistic approximation to the atmosphere, the inhomogeneous part must be multiplied by a suitable weighting function, since the chemical contribution only extends over a finite altitude regime. We also note that at each fixed altitude the driving force must tend asymptotically to zero in the Poincare sense as $t\to\infty$.

The solution of (5.1)-(5.4) is obtained by superposition. We choose a suitable function θ_1 (t, z) which satisfies the initial conditions and is damped in time. For example, set

$$\theta_1(t, z) = -(\gamma - 1) \beta k_f t e^{-\sqrt{2} t c} e^{-3z/2}$$
 (5.5)

Observe that (5.1) is satisfied and

$$M[\theta_1] = 2\sqrt{2} C (\gamma - 1) Bk_f e^{-\sqrt{2} tc} e^{-3z/2}$$

Since M[] is a linear operator, (5.1)-(5.4) may be reformulated as

$$\theta(t, z) = \theta_1(t, z) + \theta_2(t, z)$$
 (5.6)

where θ_2 (t, z) satisfies

$$M[\theta_2(t, z)] = w(t, z) - 2\sqrt{2}C(\gamma - 1)Bk_f e^{-\sqrt{2}tc}e^{-3z/2},$$
 (5.7a)

and

$$\theta_2(0, z) = \theta_{2,t}(0, z) = 0.$$
 (5.7b)

The solution of (5.7) for $\theta_2(t, z)$ is known [cf. Lamb, 1909] and is given by

$$\theta_2(t, z) = \int_0^t W(t, z; \tau) d\tau$$
 (5.8)

where

$$W(t, z; \tau) = \int_0^{tc^{-\tau}c} \left[J_0 \left(\frac{1}{2} \sqrt{(tc - \tau c)^2 - \eta^2} \right) \right] \cdot Q(\tau, z, \eta) d\eta$$
 (5.9)

and

$$Q(\tau, z, \eta) = [\varphi(\tau, z + \eta) + \varphi(\tau, z - \eta)]/2c^{2}$$
 (5.10)

with

$$\varphi(\tau, z) = w(\tau, z) - 2\sqrt{2}c(\gamma - 1) \beta k_f e^{-\sqrt{2}tc} e^{-3z/2}$$

Although (5.5) and (5.8)-(5.10) provide an exact solution of (5.1)-(5.4), this solution is complicated and yields quantitative information only through numerical calculations. The results of these calculations are given in the following sections.

A solution of (5.1)-(5.4) can also be obtained using series techniques. The result is a somewhat rapidly convergent infinite series whose terms involve products of powers (- k_f te^{-z})ⁿ and Young's functions [Young, 1912], a special case of Lommel functions. Since the series was not used to obtain physical results, it is not presented here.

From (4.12)-(4.13) we deduce the first order terms:

$$T(t,z) = e^{z/2} \theta(t,z)$$

$$u_2(t,z) = -\int_{z_s}^{z} \frac{\partial}{\partial t} \left[\frac{T}{\gamma - 1} + \beta \alpha \right] dz$$

where z_s is at the earth surface and

$$\rho(t,z) = \int_0^t \left[u_2 - \frac{\partial u_2}{\partial z} \right] dt .$$

VI. COMPUTING

The core of the numerical problem is evaluation of the integral expressions (5.8) and (5.9)

Evaluation of the above integrals was done numerically using Euler's method:

$$\theta(t,z) = \sum_{i=0}^{N} W_i(t,z,\tau_i) \Delta \tau \qquad (6.1)$$

where $\triangle \tau = t/N$ and $\tau_i = i \triangle \tau$.

Similarly,

$$W = \sum_{j=0}^{M} \left[J_0 \left(\frac{c}{2} \sqrt{(t - \tau_i)^2 - \left(\frac{\eta_j}{c} \right)^2} \right) \right] Q(\tau_i, z, \eta_j) \triangle \eta$$
 (6.2)

where

$$\Delta \eta = (\mathbf{t} - \tau) \mathbf{c}/\mathbf{M}$$
$$\eta_{\mathbf{i}} = \mathbf{j} \Delta \eta$$

The Bessel function was evaluated by numerical integration to at least five significant figures. Accuracy of the routine was checked against tables in the handbook of Chemistry and Physics.

The size of the integration mesh was decreased until the results became invariant to further decreases of mesh size.

The above procedure works quite well for short or medium times. If the integration steps are kept small for longer times, then computing becomes excessive. Conversely, if the number of intervals is kept constant, then accuracy suffers. Also, it is desirable to observe how the perturbation profile develops with time. We thus break up the integral for θ_2 into a series of integrals as follows:

$$\theta_{2}(t,z) = \sum_{k=1}^{K} \int_{\Delta t(k-1)}^{\Delta tk} W(t_{k},z,\tau) d\tau \qquad (6.3)$$

where K is chosen such that

$$t = K \triangle t$$

Since W is a function of final time, (6.3) cannot be solved unless an additional boundary condition is imposed.

Let us examine (5.9):

The quantity $\sqrt{(tc - \tau c)^2 - \eta^2}$ is familiar from the theory of wave propagation. $(t - \tau)c$ is the distance that a wavelet has travelled in time $(t - \tau)$.

Thus the η integration goes to $c(t - \tau)$, or to the limits of the physical region being considered, provided that there is no reflection at the boundaries. Let emax be the distance from the furthest point in the region considered to the

furthest point in the reaction zone. If tc > emax, one has summed all the contributions. Defining $\triangle t \ge emax/c$, it is thus permissible to write:

$$\theta_2 = \int_0^{\Delta_t} W d\tau + \int_{\Delta_t}^{2\Delta_t} W d\tau + \cdots \int_{(n-1)\Delta_t}^{n\Delta_t} W d\tau \qquad (6.4)$$

with

$$W = \int_0^{c(k\Delta t - \tau)} J_0 Q d\eta \qquad (6.5)$$

and

$$(k-1) \Delta t \leq \tau \leq k \Delta t$$
.

The quantity $t-\tau$ ranges from zero to $\triangle t$ making the values of the Bessel function independent of k. Since the range of η is thus to, it becomes possible to compute a matrix of Bessel functions

$$MJ_0(I,J)$$

where the index I refers to $(t - \tau)$ (I) and the index J refers to η (J). Q, however, depends on the actual time elapsed, and must thus be computed for each value of k.

The integral for W is therefore approximated by:

$$W(K, I) = \sum_{J=1}^{J \text{MAX}} MJ_0(I, J) Q(K, J) \Delta \eta(J) \qquad (6.6)$$

 θ_2 is approximated by:

$$\theta_2 = \sum_{I=1}^{IMAX} \theta_I(I)$$
 (6.7)

and

$$\theta_{\mathbf{I}}(\mathbf{I}) = \sum_{\mathbf{K}=1}^{\mathbf{KMAX}} \mathbf{W}(\mathbf{K}, \mathbf{I}) \triangle \tau(\mathbf{K})$$
 (6.8)

The rate of change of temperature, or θ , is needed to evaluate the velocity. This is computed using the forward difference approximation:

$$\frac{\mathrm{d}\,\theta}{\mathrm{d}\,t} \approx \frac{\Delta\,\theta}{\Delta\,t} = \frac{\theta_{\mathrm{n}} - \theta_{\mathrm{m}}}{t_{\mathrm{n}} - t_{\mathrm{m}}} \tag{6.9}$$

The derivatives of θ_1 and α are evaluated from exact analytical expressions. The velocity is estimated by a simple numerical integration in z, taking the velocity at the earth's surface to be zero. Density deviation is estimated the same way. It should be noted that the step sizes for z were between 0.1H and 0.5H. Thus, the velocity and density estimates are generally less reliable than the temperature estimates.

VII. NUMERICAL RESULTS

At very short times a pulse is seen propagating up and down from the reaction zone. The initial pulse has the appearance of a discontinuity. Eventually the pulse passes outside the range of the computation regime, and a pseudo-steady pattern is established in which the qualitative behavior of the parameters does not change. However, the quantitative values increase to a maximum, and then decay. The development and decay of the pseudo-steady patterns are illustrated in Figures 1 through 3.

The type of behavior observed may be partially explained by analogy with a shock tube whose driven end is semi-infinite. Initially the shock passes, then a pseudo-steady state is established and eventually decays. The above analogy is incomplete, since the atmosphere also behaves like an elastic medium resulting in the establishment of something like a standing wave pattern. However, an acoustic treatment would be incorrect because the gravity restoring force is important, and because the reaction generates pulses all of one sign, either compression or rarefaction. Perhaps another analogy is a spring with weights at the end. When weights are suddenly added or removed, wave patterns are set up in the spring. Now, consider that a series of weights are added or removed in succession. Also, let the spring be very stiff near the bottom, becoming progressively more elastic toward the top.

Figure 1 shows a series of θ profiles. The length of the reaction zone is 0.5 H, the reaction is exothermic, and the nondimensional rate constant is 0.01. Figure 1 shows buildup of the θ profile. The reaction zone was chosen to be 0.5 H deep, the reaction was exothermic, and the nondimensional rate constant

was 0.01. The reference value, ω_R , equals $10^{-2}\,\mathrm{sec}^{-1}$; thus time is given in units of 100 seconds. The characteristic time of the reaction is defined as the point where $k_F t = 1$. Strictly speaking, one needs $k_F \rho^{(0)} t = 1$, but $\rho^{(0)} = 1$ at the bottom of the reaction zone. Since $\rho^{(0)}$ drops off exponentially with altitude, while k_F remains constant, it follows that the characteristic time increases exponentially with altitude until the end of the reaction zone is reached. It may be shown that

$$k_F t = k_F^* t^*$$

where the starred quantities are dimensional. For k_F^* = 10^{-2} sec⁻¹ the characteristic time is 10^2 in non-dimensional units, or 10^4 sec = 2.8 hrs. At z = 0.5 H, the characteristic time becomes 4.6 hrs.

The absolute maximum value of θ occurs at z=0 and grows with time. A relative maximum is found at z=10, this secondary maximum also grows with time. Essentially, θ follows a Bessel function type of altitude pattern as might be expected. The growth of θ at z=0 and at z=10 is presented in Figures 2 and 3. Figure 4 shows development of the temperature profiles.

Outside the reaction zone the velocity equation becomes:

$$\frac{\partial \mathbf{u}}{\partial \mathbf{z}} = \frac{-1}{\gamma - 1} \frac{\partial \mathbf{T}}{\partial \mathbf{t}}$$

During the buildup of temperature we have

$$\frac{T6}{6}$$
 > 0

everywhere except in a small region near six scale heights. One may conclude that velocity is generally negative during the buildup phase, especially above 8 scale heights. This conclusion is indeed correct.

Physically we know that subsidence in an isothermal atmosphere results in heating. Conversely, an upward motion gives rise to cooling. This is precisely the kind of behavior observed, so we may conclude that the result is physically consistent. Similarly, convergency of velocity results in compression while divergence gives rarefaction. These combined effects are illustrated in Figure 5 which, incidentally is for an endothermic reaction, five scale heights deep.

If we had an adiabatic lapse rate, then physical argument would lead us to expect disappearance of the most pronounced part of the temperature wave. However, the velocity wave would not disappear; consequently, a temperature effect would become visible at an altitude where the lapse rate became less than adiabatic. If the atmosphere has an inversion, then the temperature wave would be especially pronounced.

Several special cases are discussed below.

The first case to be considered is a severe rain storm. Condense saturated air at 5 km altitude (270 degrees Kelvin) until 25% of it is ice, using a reaction characteristic time of 3 hours and a reaction depth of half of a scale height. The mixing ratio, X_0 is 0.002, and the non-dimensional enthalpy, B, is just under 200. The reaction is of course exothermic. Since the extent of a rainstorm,

or even a hurricane, is not large enough to really warrant a one-dimensional approximation, the storm was assumed to be approximated by a line source centered at 6 H below ground level. The above approximation results in a $\frac{1}{R}$ amplitude fall-off relative to the pure one dimensional case. It is realized that the two-dimensionality correction employed is quite arbitrary, and that agenuine two-dimensional solution of the atmospheric equations of motion is needed. However, the results, shown in Figure 4, seem to agree reasonably well with experimental observations, as shown by Eberstein and Theon (1971).

Our calculations were taken to ten scale heights above the bottom of the reaction zone. Whereas the ten scale height limit was chosen quite arbitrarily, there are nonetheless compelling reasons for limiting the vertical extent to which computations are carried out. Firstly, the one-dimensional assumption becomes ever less meaningful as the vertical extent of space is increased.

Secondly, the temperature perturbation involves an exponential in altitude, i.e.,

$$T = \theta e^{z/2}$$

with the consequence that small errors in θ can give rise to large temperature errors as z becomes large. Also, the non-dissipation and isothermal atmosphere assumptions lose validity as one considers effects propagating over large distances. A more detailed and comprehensive theory is needed to study the effect of severe thunderstorms or hurricanes on regions in the ionosphere and above. However, the present analyses illustrates that such effects would

definitely be expected. This conclusion is borne out by experimental observations. Thus Bauer (1958) has shown a correlation between hurricane passage and electron concentration in the \mathbf{F}_2 layer of the ionosphere. More recently, Davies and Jones (1971) have reported association between ionospheric disturbances in the \mathbf{F}_2 region and severe thunderstorms. Davies and Jones believe that the ionosphere is perturbed by infrasonic disturbances generated by mechanical motions of the thunderstorms, but are not due to buoyancy oscillations. We would suggest that heat released by the storm induces vertical motion, thus influencing the electron concentration and transmission properties of the \mathbf{F}_2 layer.

While the ionosphere is outside our quantative reach, the ozonosphere is relatively accessible. Reed (1950) suggests qualitative explanations in terms of vertical and horizontal motions for correlations between ozone concentration and weather phenomena. The existence of an ozone-weather relationship is described as well known. Reed specifically considers subsidence at high altitudes as one of the means by which ozone concentration is increased. Our model predicts that a severe storm will cause considerable subsidence at ozone altitudes, in agreement with Reed's suggestion.

At the time of computation the velocity and density information were considered to be of secondary importance. A rather crude z mesh was thus used to save computer time, with the result that the quantative velocity profiles must

be considered approximate. Nonetheless, we are confident that a severe storm causes large and sustained subsidence at ozone altitudes. It would be very interesting to use a fine vertical mesh computation or a more sophisticated mathematical technique to obtain a quantitative estimate of the ozone concentration change.

One might also consider the effect of changes in the ozone layer on the upper atmosphere. A reaction having the thermal properties of ozone dissociating to molecular oxygen was considered. The reaction characteristic time was taken to be 20 minutes. This results in a maximum perturbation at approximately 4 hours. The type of perturbation profile attained is shown in Figure 5. A 2 degree Kelvin cooling at the first maximum seems quite reasonable (Krueger, 1971). At the second maximum (9 H above the bottom of the reaction zone) the temperature change is 15 degrees. The associated density perturbation is 6%, and vertical velocity is 40 cm/sec at 10 minutes, going to 5 cm/sec at 4 hours. Since the second maximum is above 90 km where large atmosphere variations are frequently found, one must conclude that upper atmosphere effects of ozone variations are not very important.

A very different conclusion is reached regarding the effects of aurorae on the upper atmosphere. Insofar as a rather large amount of heat is rapidly released in a small altitude regime, the thermodynamic effect of aurorae is very similar to that of a severe thunderstorm or hurricane. The expected behavior is thus generally similar to that shown in Figure 4. If one takes an initial heating rate of 25 ergs/cm²-sec and a reaction characteristic time of 20 minutes, with heating concentrated in half a scale height, then the quantitative deviations are approximately the same as those snown in Figure 4. If the mean heating rate is 25 ergs/cm2-sec, then the deviations become twice as large. According to D. Heath (1971) auroral heating rates vary between 10 ergs/cm²-sec and 100 ergs/cm²-sec with heating concentrated in less than one scale height. Corresponding characteristic times vary between 10 minutes and 100 minutes. Since our solution is linear, it becomes possible to estimate upper atmosphere effects anywhere in this range. The maximum temperature deviation predicted is then in the order of 500 degrees at some 200 km for the case of a mean heating rate of 100 ergs/cm²-sec. The actual value of 500 degrees must, of course, not be taken too seriously, especially since large heat releases, and associated large accelerations violate some of the assumptions on which our solution is based. Nonetheless, the theory does predict a large temperature increase well above the main auroral display altitude.

VIII. CONCLUSIONS

A one-dimensional model for impulsive heat release in the atmosphere has been developed. The theory described is intended as a simple tool to study the effects of impulsive heat release. Such heating, or cooling, is found to cause large disturbances at higher altitudes.

The inclusion of a second space variable and additional mathematical modeling of heat sources is needed. Among existing solutions including more than one space dimension are acoustic waves, internal gravity waves, and tidal waves. However, all three above mentioned waves are special restricted solutions to the atmospheric equations. Specifically, acoustic and gravity waves have sinusoidal space and time behavior. Tidal waves have a sinusoidal time behavior and a spatial behavior described in terms of Hough functions. The above theories are quite good for evaluating the long distance propagation of periodic disturbances. However, these theories may not readily be employed to study the short distance effects of impulsive heat releases in the atmosphere. Our one-dimensional theory has been an initial step toward an analytical solution to the problem of impulsive heat releases in the atmosphere. Thunderstorms, hurricanes, chemical reactions, and aurorae have been discussed 2 important natural sources of impulsive heat release.

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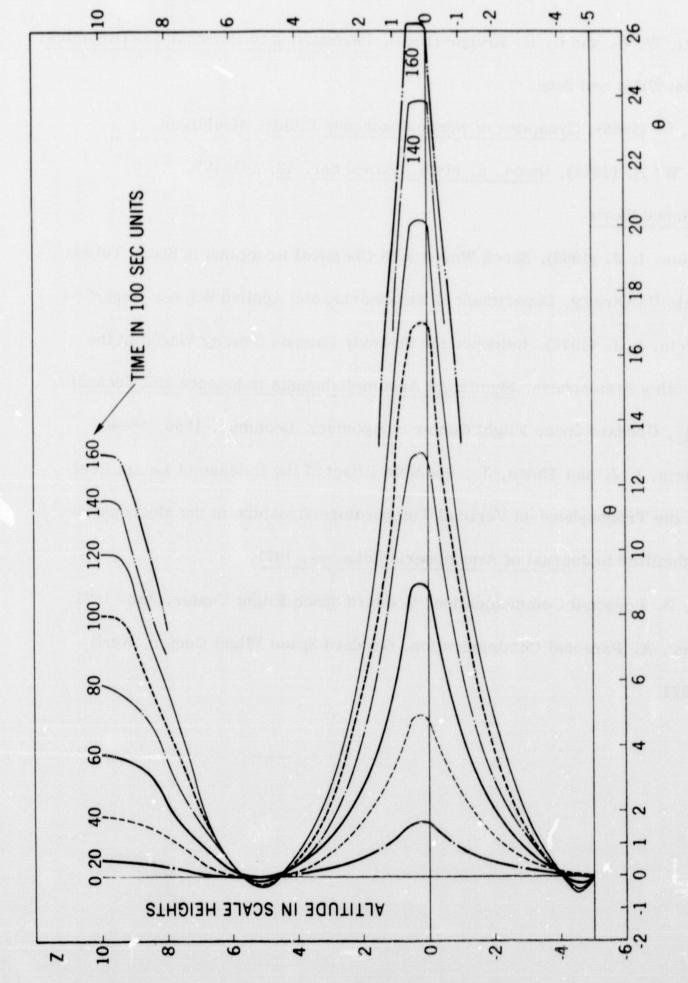
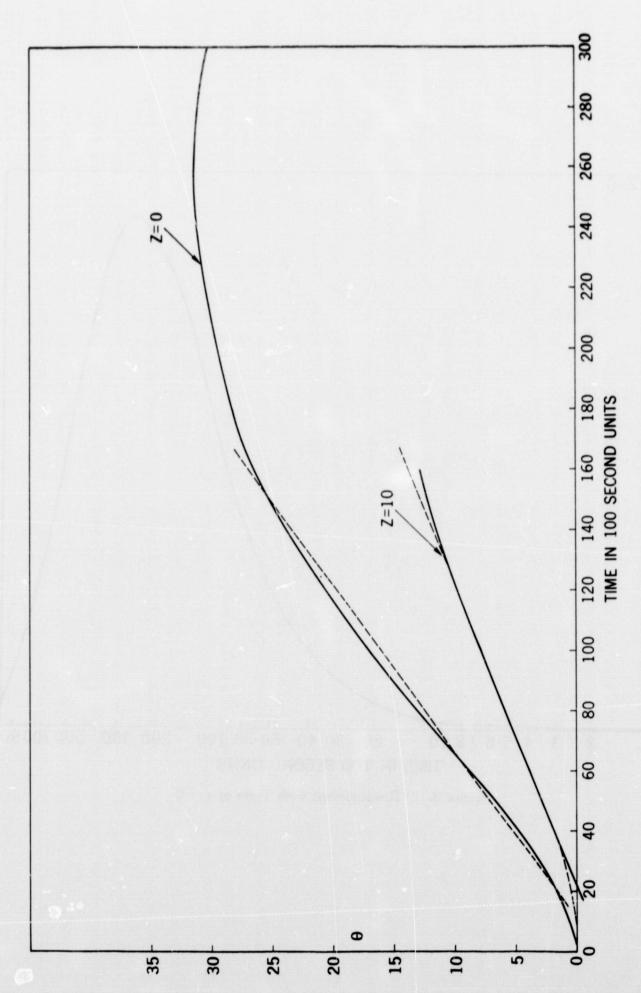


Figure 1. θ Profiles



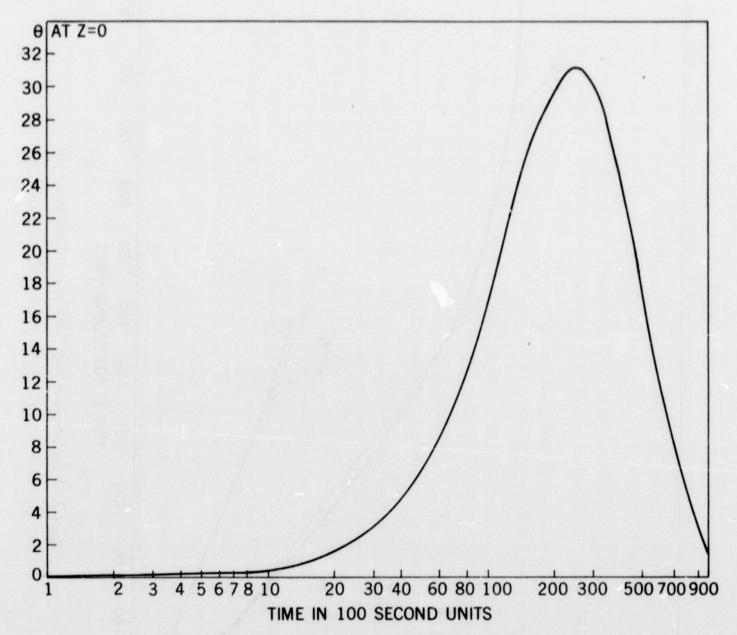


Figure 3. θ Development with Time at z = 0

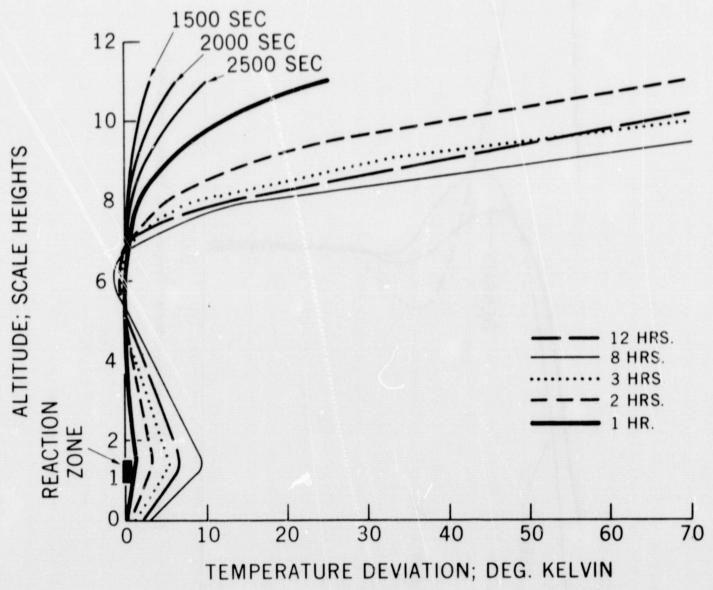


Figure 4. Temperature Deviation for Storm (3 hr Half-Life at z = 1 H)

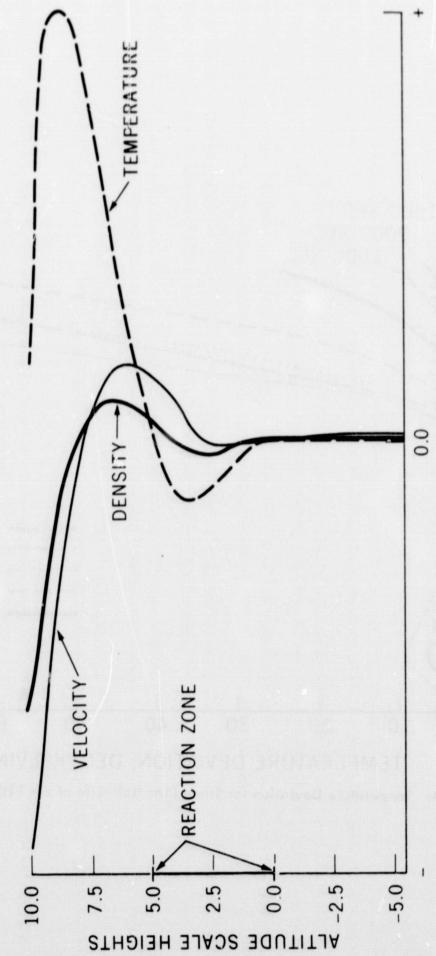


Figure 5. Profiles of Perturbation Temperature, Velocity and Density